Amirkabir Journal of Civil Engineering

Amirkabir J. Civil Eng., 53(1) (2021) 61-64
DOI: 10.22060/ceej.2018.14346.5629

Kinetic Constant Modeling of Zn(II) Ion Removal from Synthetic Wastewater by Gene Expression Programing

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ABSTRACT: The separation of ions from wastewater and environments such as hydrometallurgy has been a major challenge in the development of ion flotation in recent years. Few studies have been carried out on the kinetics of metal ion removal by ion flotation. In this study, a new model using the gene expression programming (GEP) method is proposed to predict the kinetic constant of zinc ion removal (k-Zn(II)) from synthetic wastewater with sodium dodecyl sulphate as a collector. The efficiency of ion flotation depends on both the amount of ion removal and water removed during the process. In this regard, the water removal kinetics constant (k-W) was also investigated. The effect of important parameters on k-Zn(II) and k-W including the ratio of SDS/Zn(II), the activity coefficient, and the pH were investigated. The values of R^2, RMSE, and VAF of the GEP models for the testing data for k-Zn(II) were 0.98, 0.66, and 98.9 and for k-W, they were 0.94, 0.004, and 0.93, respectively. The results indicate the high performance of GEP models for the prediction of k-Zn(II) and k-W. The sensitivity analysis of GEP models showed that k-Zn(II) and k-W are more sensitive to the pH and ratio of SDS/Zn(II), respectively.

Review History:

Received: 4/21/2018
Revised: 5/9/2018
Accepted: 7/7/2018
Available Online: 7/14/2018

Keywords:

Ion flotation, Kinetics
Zn(II) ion removal
Water removal
Sensitivity analysis

1. INTRODUCTION

An increase in the world's population has led to an increase in industrial production, which produces a large amount of industrial wastewater. Flotation is widely used in environmental processes to remove heavy metal ions from industrial wastewater and recover metal ions from solutions. Ion flotation has been successfully used for the recovery of metals such as copper, chromium, cadmium, nickel, zinc, silver, germanium, and gold. Ion flotation is a physicochemical process that is influenced by parameters such as the type and concentration of chemical reagents, pH, activity coefficient, air flow rate, agitation speed, cell type, and bubble size [1].

By evaluating the effective parameters on the kinetics of ion flotation, the required time for designing the process to achieve optimal recovery can be investigated. The kinetics of the process can be increased by optimizing different parameters. A few studies have proposed a model for ion flotation kinetics [2]. So far, there is no general model that includes all or most of the parameters that control the process efficiency and the proposed kinetics models of ion flotation are experimental [3]. The ion flotation process is a complex physicochemical method that cannot be modeled by simple regression modeling methods. In this regard, the gene expression programming (GEP) method was used to obtain a mathematical relationship for the prediction of the kinetic constant of Zn(II) ion removal.

A few studies have evaluated water removal during the ion flotation process. The ion flotation efficiency depends on both Zn(II) removal and water removal [4]. In this study, kinetic constant modeling of Zn(II) ion and water removal from synthetic wastewater by GEP was proposed.

2. MATERIAL AND METHOD

The ionic salts of zinc sulphate ($(Zn(SO_4)_2.7H_2O$) and the collector of sodium dodecyl sulphate (SDS) were obtained from Merck and the frother of Dowfroth 250 (DF250) was obtained from Dow Chemical. The solution pH was adjusted using hydrochloric acid (HCl) and caustic soda (NaOH) (Merck). The initial ion concentration of 10 mg/L Zn(II) was used in the experiments. A Denver-type laboratory flotation cell with a constant capacity of 1 L was used.

The Zn(II) removal percentage (*R*) was calculated by Eq. (1). The simple zero-order, first-order, second-order equations (Eq. (2)) and the empirical equation proposed by Rubin et al. (Eq. (3)) were used in the kinetic studies of ion flotation [1].

$$R(\%) = (1-(c_r/c_i)\ \times 100 \tag{1}$$

$$\frac{dc}{dt} = -kc^n \tag{2}$$

$$\frac{dc}{dt} = -\frac{c_i}{c_i - c_r} k(c - c_r)^n \tag{3}$$

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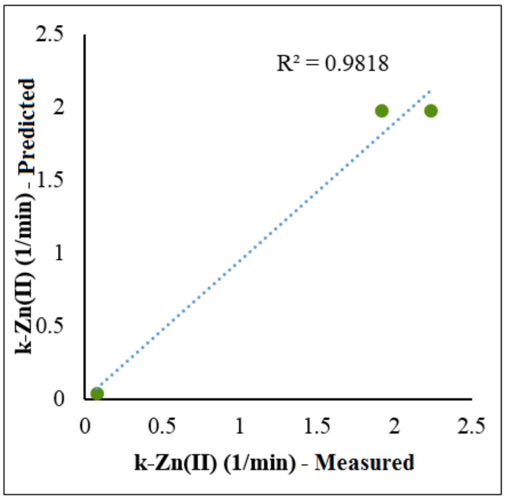

Fig. 1. Predicted k-Zn(II) by GEP in the testing process vs. actual measurement.

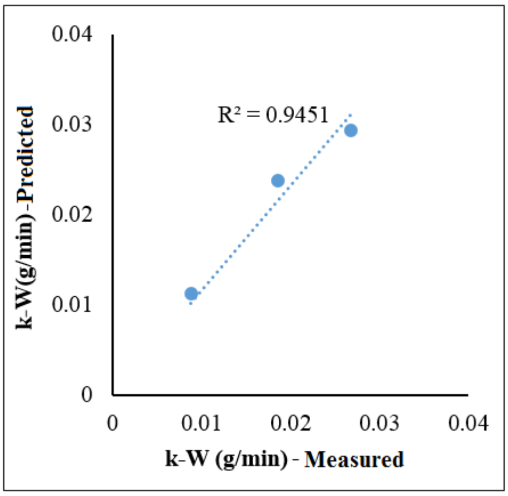

Fig. 2. Predicted k-W by GEP in the testing process vs. actual measurement

where k is the rate constant, n is the order of flotation, c_i and c_r, c are the concentrations at time 0, infinite time, and time t, respectively. To develop a kinetic model, the first-order equation was used as follows:

$$\frac{dc}{dt} = -\frac{c_i}{c_i - c_r} k(c - c_r) \Rightarrow k \propto (pH, SNR, AC) \qquad (4)$$

where pH, SNR, and AC are the pH solution, the ratio of SDS/Zn(II), and activity coefficient, respectively. GeneXproTools 5.0 software was used for modeling.

3. GENE EXPRESSION PROGRAMMING

GEP is a new population-based evolutionary algorithm. It is a useful method to develop a mathematical equation between input parameters for the prediction of output with high accuracy and low estimation error. GEP can check all search spaces and detect the global optimum without getting stuck in a local minimum. GEP is the improvement of the genetic algorithm (GA) and genetic programming (GP) which improves problems such as overfitting, creating infeasible solutions, and problems related to using genetic operators on chromosomes. Details about the GEP algorithm can be found in the literature [5].

4. RESULTS AND DISCUSSION

In this section, mathematical equations were developed using the GEP method in the form of the kinetic constant of Zn(II) ion removal/water removal= f (pH, SNR, γ). All input data were normalized before modeling in the range of 0 and 1. Then, the datasets were randomly divided into training and testing sections. The mathematical operators of +, —, × , /, Ln, Exp, Log, Sqrt, ^2, ^3, 3Rt, Sin, Cos, Tan, Atan were used in GEP modeling by the trial-and-error procedure. The root mean square error (RMSE) is assigned as the fitness function to investigate the generated chromosome fitness. The optimum architecture of chromosomes was specified during modeling with the evaluation of various conditions of chromosome architecture. The optimum values of head size and genes were obtained 8, 3 for k-Zn(II) and 9, 3 for k-W, respectively. Finally, the multiplication function was used to link the genes.

Figs. 1 and 2 show the measured values of the kinetic constant of Zn(II) ion removal (k-Zn(II)) and the water removal (k-W) versus the predictions of GEP models in the testing processes, respectively. The results show that the kinetic constant predicted values using GEP models are closer to their measured values. The values of R^2, RMSE, and VAF of the GEP models for the testing data for k-Zn(II) were 0.98, 0.66, and 98.9 and for k-W, they were 0.94, 0.004, and 0.93, respectively. The results indicate the high performance of GEP models for the prediction of k-Zn(II) and k-W.

5. CONCLUSIONS

The process kinetics of ion removal is one of the effective parameters on the efficiency of ion flotation. The efficiency of ion flotation should be investigated by considering both Zn(II) removal and water removal value during the process. Thus, in this study, the kinetics of water removal was also evaluated. Predictive models of the kinetic constant of Zn(II) ion removal and water removal were proposed by considering the effective parameters including pH, the ratio of SDS/Zn(II), and activity coefficient. The results showed that the proposed GEP models can be applied to predict the rate constant of Zn(II) ion removal and water removal with reasonable error.

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HOW TO CITE THIS ARTICLE

F. S. Hoseinian, B. Rezai, E. Kowsari, Kinetic Constant Modeling of Zn(II) Ion Removal from Synthetic Wastewater by Gene Expression Programing, Amirkabir J. Civil Eng., 53(1) (2021) 61-64.

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